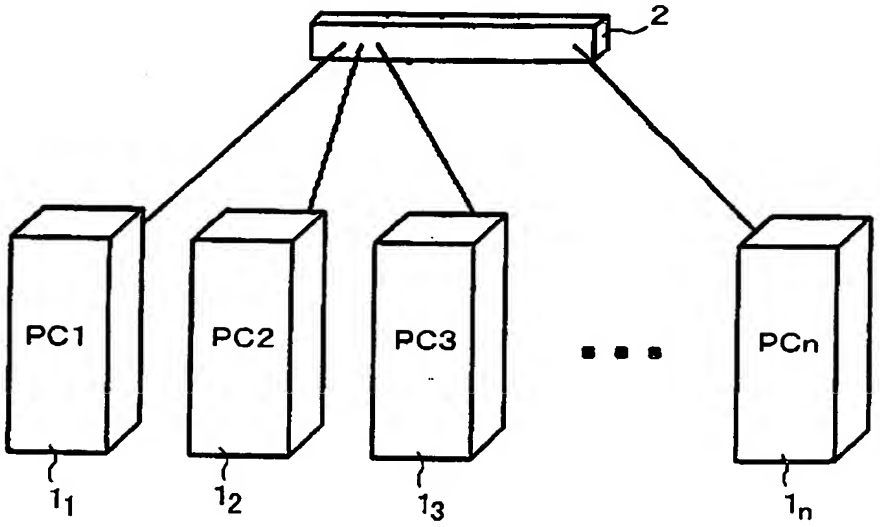
2
PC1
PC2
PC3
PCn
1 1
1 2
1 3
1 n

FIG. 1

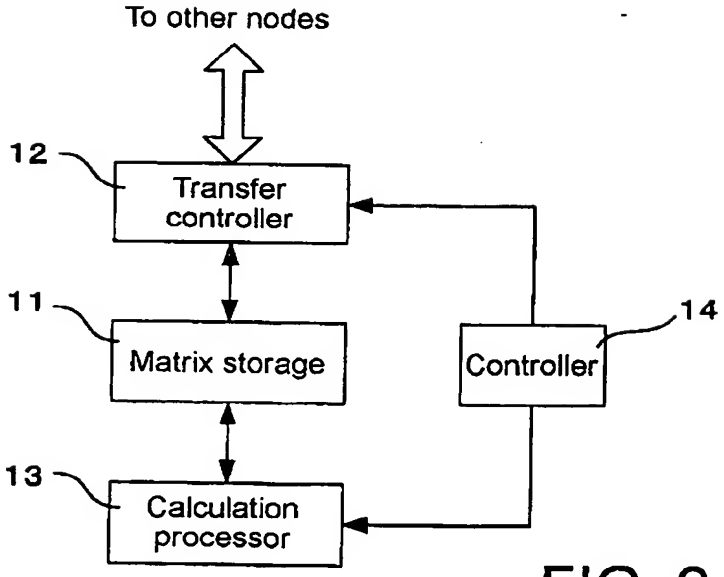
To other nodes
12
Transfer controller
11
Matrix storage
14
Controller
13
Calculation processor

FIG. 2

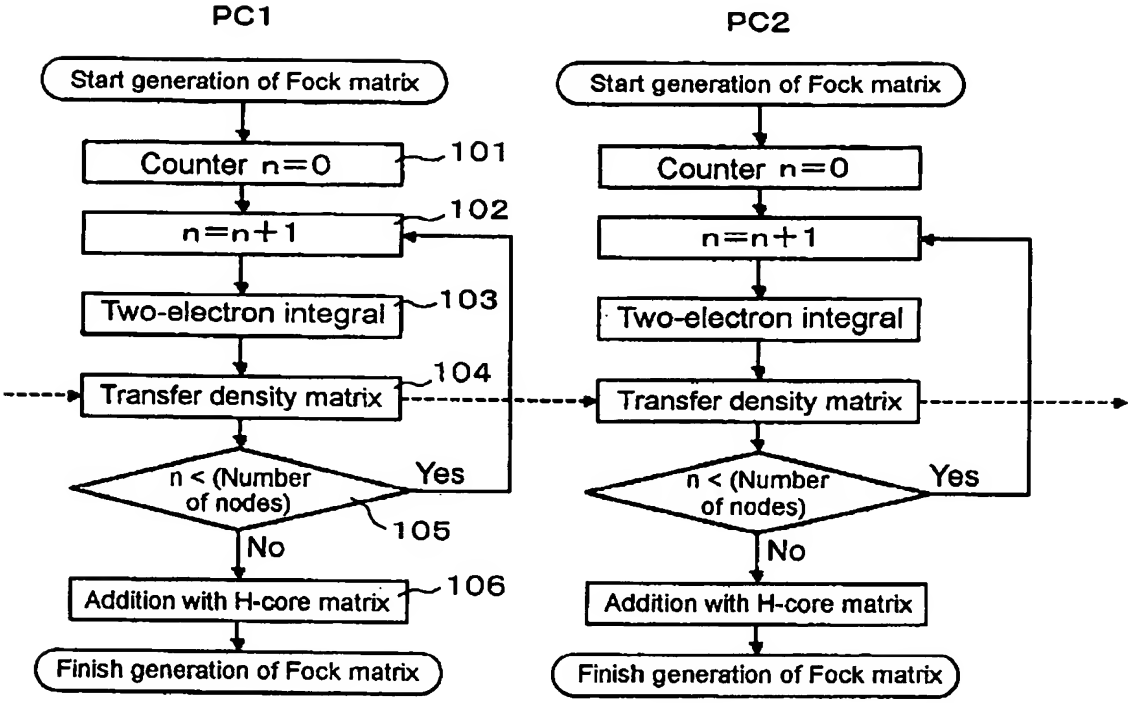
PC1
PC2
Start generation of Fock matrix
Counter n=0
n=n+1
Two-electron integral
Transfer density matrix
n < (Number of nodes)
Yes
No
Addition with H-core matrix
Finish generation of Fock matrix
101
102
103
104
105
106

FIG. 3

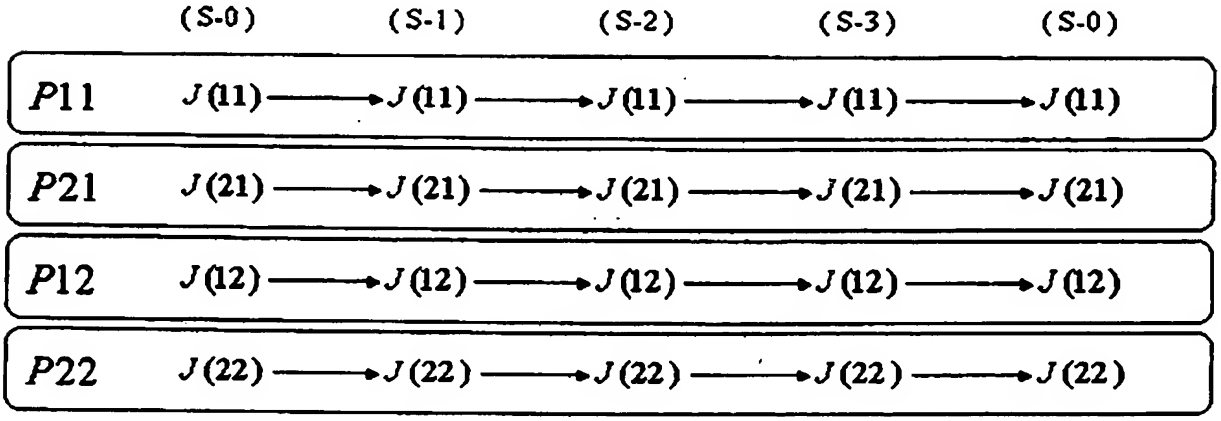
(S-0)
(S-1)
(S-2)
(S-3)
(S-0)
P11
P21
P12
P22
J(11)
J(21)
J(12)
J(22)

FIG. 4

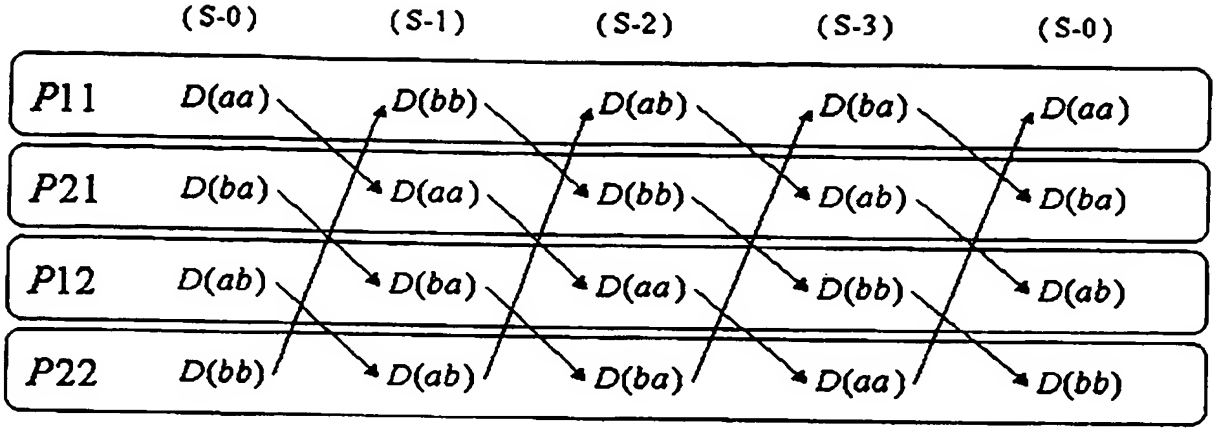

FIG. 5

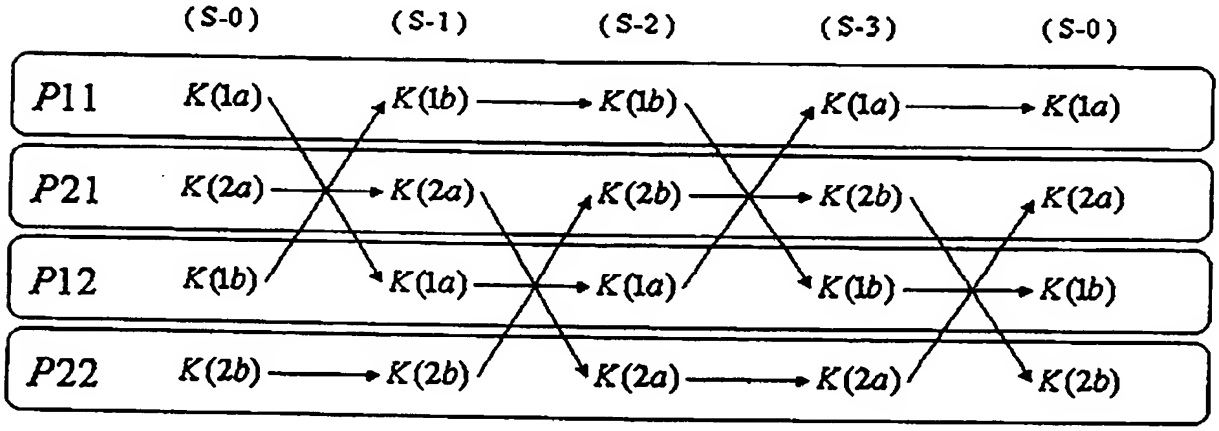

FIG. 6

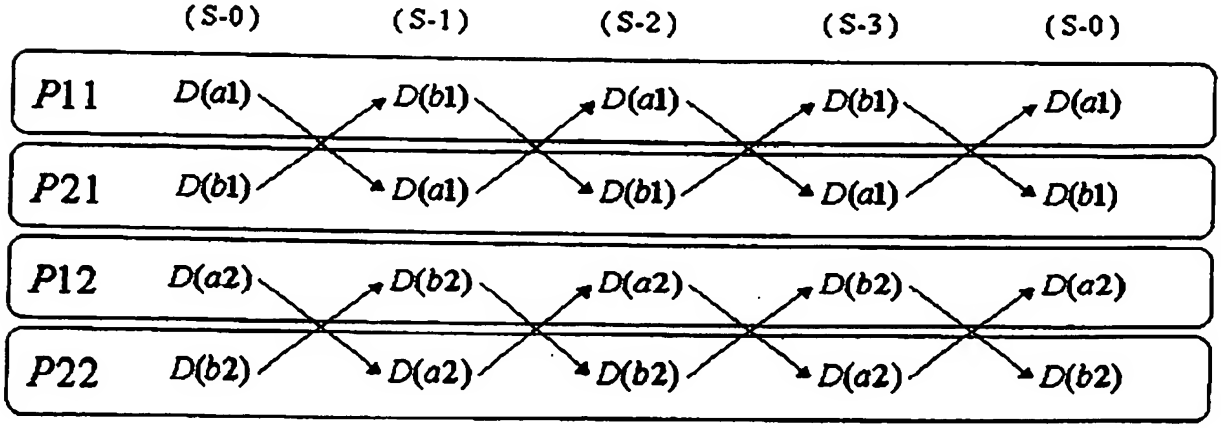

FIG. 7

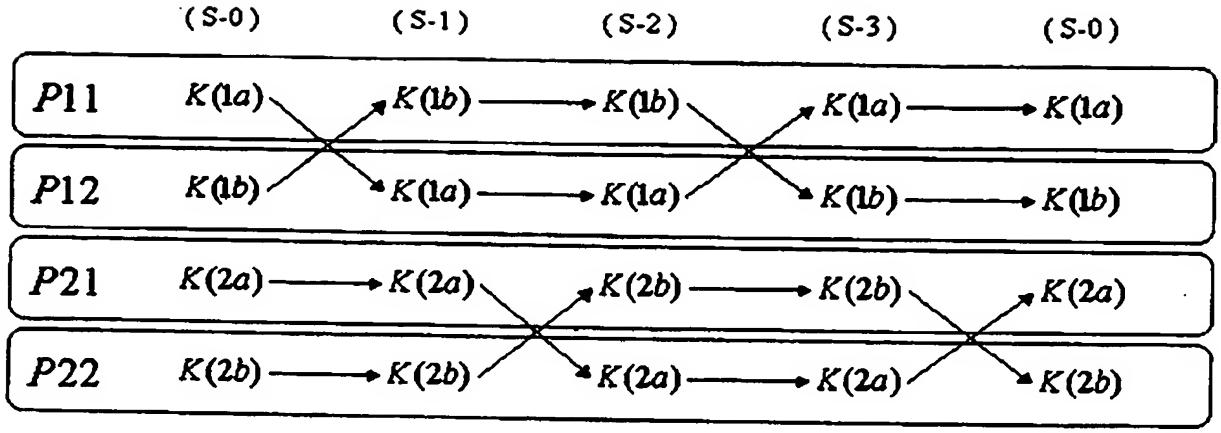
(S-0)
(S-1)
(S-2)
(S-3)
(S-0)
P11
P12
P21
P22
K(1a)
K(1b)
K(2a)
K(2b)

FIG. 8

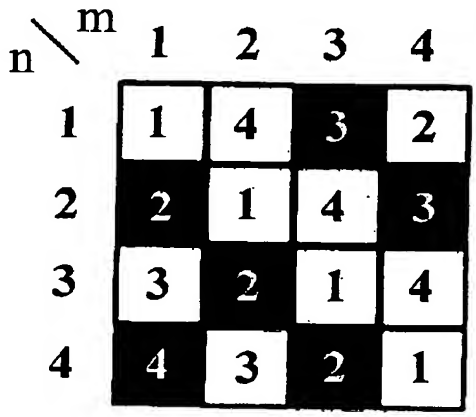
m
n
1 2 3 4
1 1 4 3 2
2 2 1 4 3
3 3 2 1 4
4 4 3 2 1

FIG. 9

n \ m	1	2	3	4	5	6	7	8	9
1	1	9	8	7	6	5	4	3	2
2	2	1	9	8	7	6	5	4	3
3	3	2	1	9	8	7	6	5	4
4	4	3	2	1	9	8	7	6	5
5	5	4	3	2	1	9	8	7	6
6	6	5	4	3	2	1	9	8	7
7	7	6	5	4	3	2	1	9	8
8	8	7	6	5	4	3	2	1	9
9	9	8	7	6	5	4	3	2	1

FIG. 10